

LARGE EDDY SIMULATIONS OF FIRES - FROM CONCEPTS TO COMPUTATIONS

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1 Introduction

The idea that the dynamics of a fire might be studied using digital computers probably dates back to the beginnings of the computer age. The concept that a fire requires the mixing of a combustible gas with enough air at elevated temperatures is well known to anyone involved with fire. Graduate students enrolled in courses in fluid mechanics, heat transfer, and combustion have been taught the equations that need to be solved for at least as long as computers have been around. What is the problem? The difficulties revolve about three issues: First, there are an enormous number of possible fire scenarios to consider. Second, we do not have either the physical insight or the computing power (even if we had the insight) to perform all the necessary calculations for most fire scenarios. Finally, since the "fuel" in most fires was never intended as such, the data needed to characterize both the fuel and the fire environment may not be available.

In order to make progress, the questions that are asked have to be greatly simplified. To begin with, instead of seeking a methodology that can be applied to all fire problems, we begin by looking at a few scenarios that seem to be most amenable to analysis. Hopefully, the methods developed to study these "simple" problems can be generalized over time so that more complex scenarios can be analyzed. Second, we must learn to live with idealized descriptions of fires and approximate solutions to our idealized equations. These idealized descriptions have to be based on the kind of incomplete knowledge of fire scenarios that is characteristic of real fires. Finally, the methods should be capable of systematic improvement. Thus, as our physical insight and computing power grow more powerful the methods of analysis can grow with them.

The "Large Eddy Simulation" (LES) technique developed at NIST over a nearly two decade period is our attempt to carry out the conceptual program outlined above. The phrase refers to the description of turbulent mixing of the gaseous fuel and combustion products with the local atmosphere surrounding the fire. This process, which determines the burning rate in most fires and controls the spread of smoke and hot gases, is extremely difficult to predict accurately. This is true not only in fire research but in almost all phenomena involving turbulent fluid motion. The basic idea behind the use of the LES technique is that the eddies that account for most of the mixing are large enough to be calculated with reasonable accuracy from the equations of fluid mechanics. The hope (which must ultimately be justified by appeal to experiments) is that small scale eddy motion can either be crudely accounted for or ignored.

The equations describing the transport of mass, momentum, and energy by the fire induced flows must be simplified so that they can be efficiently solved for the fire scenarios of actual interest. The general equations of fluid mechanics describe a rich variety of physical processes, many of which have nothing to do with fires. Retaining this generality would lead to an enormously complex computational task that

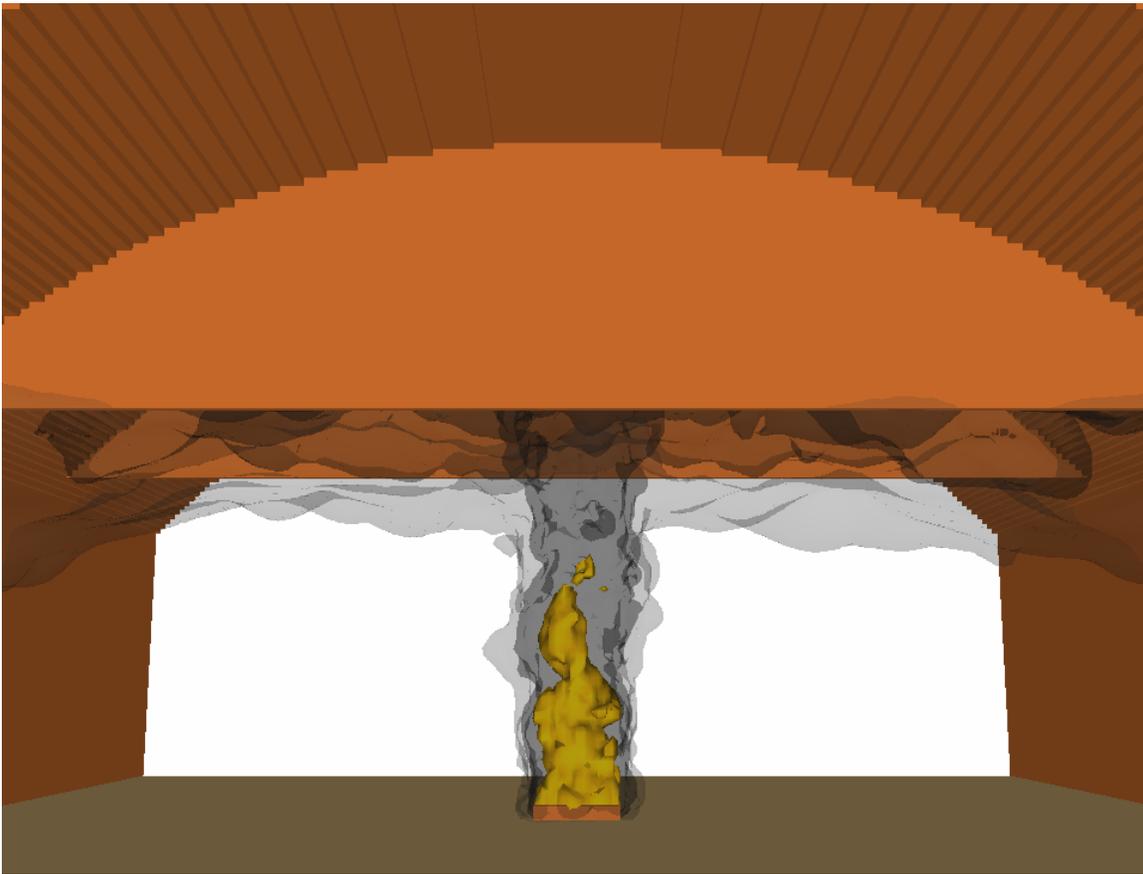


FIGURE 1: Snapshot of a simulation of 3 m square jet fuel fire in a 22 m high and 45 m wide aircraft hangar. Contours corresponding to the mean flame temperature maximum and the highest temperature non-burning region are shown.

would shed very little additional insight on fire dynamics. The simplified equations, developed by Rehm and Baum [1], have been widely adopted by the larger combustion research community, where they are referred to as the “low Mach number” combustion equations. They describe the low speed motion of a gas driven by chemical heat release and buoyancy forces.

The low Mach number equations are solved on the computer by dividing the physical space where the fire is to be simulated into a large number of rectangular cells. In each cell the “state of motion”, i.e. the gas velocity, temperature, etc. are assumed to be uniform; changing only with time. The computer then computes a large number of snapshots of the state of motion as it changes with time. Figure 1 shows one such snapshot of a hangar fire simulation. Clearly, the accuracy with which the fire dynamics can be simulated depends on the number of cells which can be incorporated into the simulation. This number is ultimately limited by the computing power available to the user. Present day computers limit the number of such cells to at most a few million. This means that the ratio of largest to smallest eddy length scales that can be resolved by the computation (the “dynamic range” of the simulation) is roughly $100 \sim 200$. Unfortunately, the range of length scales that need to be accounted for if all relevant fire processes are to be simulated is roughly $10^4 \sim 10^5$. Much of the discrepancy is due to the fact that the combustion processes that release the energy take place at length scales of 1 mm or less.

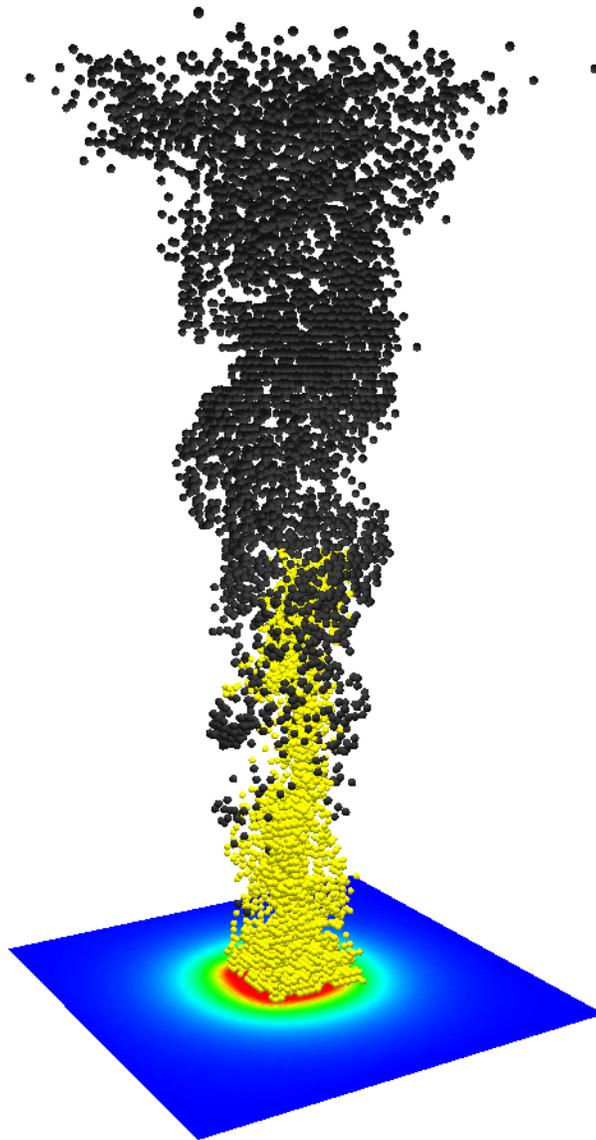


FIGURE 2: Snapshot of isolated plume structure showing burning elements (light color), burnt out combustion products (dark color), and radiation heat flux contours to fuel bed.

2 Fire Plumes

The idea that different physical phenomena occur at different length and time scales is central to an understanding of fire phenomena, and to the compromises that must be made in attempting to simulate them. The most important example is an isolated fire plume in a large well ventilated enclosure (see fig. 1). Simulations of scenarios of this kind are reported in refs. [2] and [3]. The fire plume is the “pump” which entrains fresh air and mixes it with the gasified fuel emerging from the burning object. It then propels the combustion products through the rest of the enclosure. The eddies that dominate the mixing have diameters that are roughly comparable to the local diameter of the fire plume. Thus, in the above simulation, the cells have to be small enough so that many (a 12x12 array in this case) are used to describe the state of motion across the surface of the fuel bed. Since the simulation also needs to include the remainder of the hangar as well, even the 3 million cell simulation shown in fig. 1 above cannot cope with the combustion

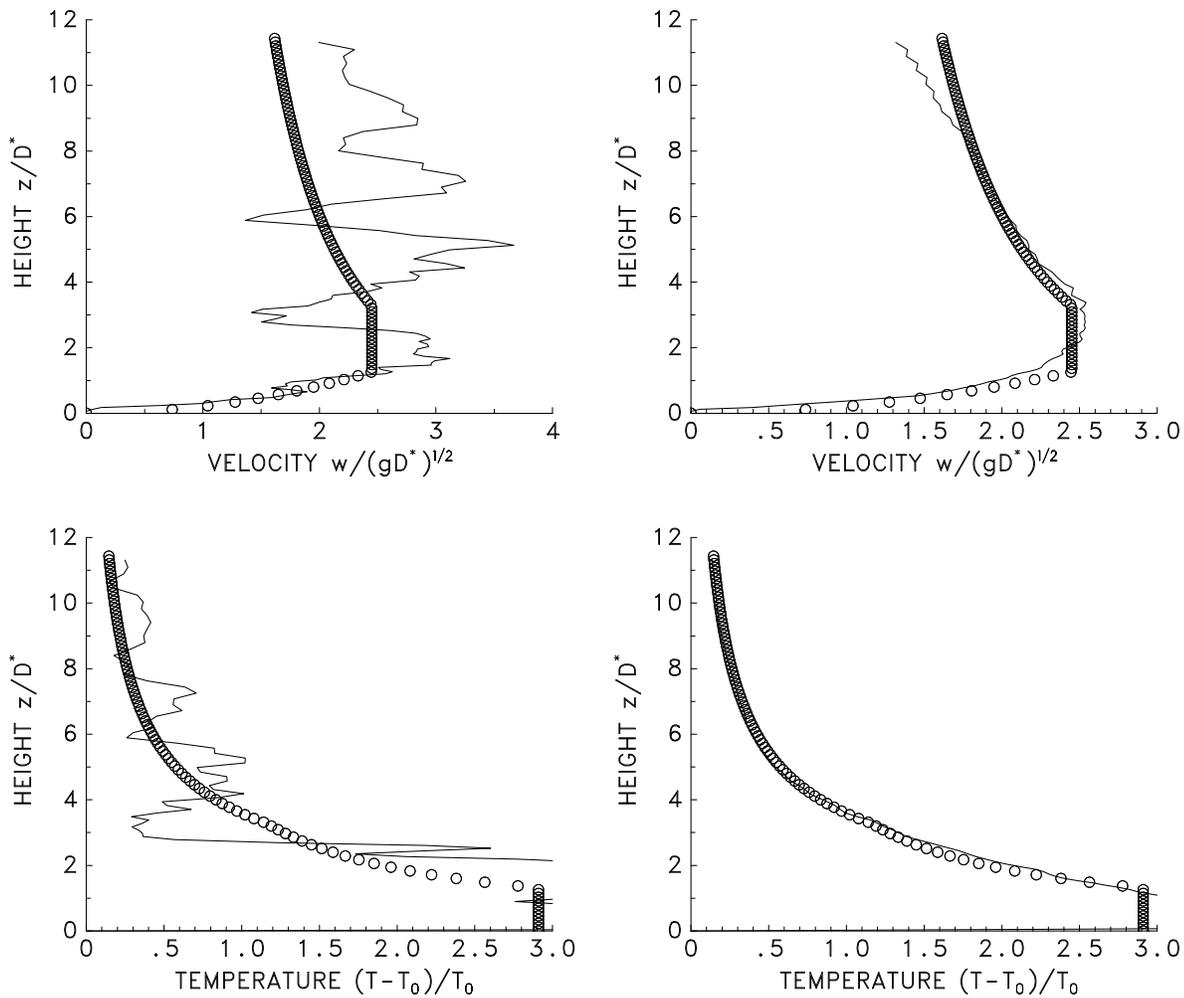


FIGURE 3: Instantaneous (left) and time-averaged (right) centerline velocity and temperature profiles for a pool fire simulation.

processes without additional modeling effort.

Physical processes like combustion that occur on scales much smaller than the individual cell size are often called “sub-grid scale” phenomena. The most important of these for our purposes are the release of energy into the gas, the emission of thermal radiation, and the generation of soot together with other combustion products. These phenomena are represented by introducing the concept of a “thermal element” [4]. This can be thought of a small parcel of gasified fuel interacting with its environment. The concept is illustrated in figure 2.

Each element is carried along by the large scale flow calculated as outlined above. As long as the fire is well ventilated, it burns at a rate determined by the amount of fuel represented by the parcel and a lifetime determined by the overall size of the fire. The lifetime of the burning element is determined from experimental correlations of flame height developed by McCaffrey (see [5]). A prescribed fraction of the fuel is converted to soot as it burns. Each element also emits a prescribed fraction of the chemical energy released by combustion as thermal radiation. This fraction is typically about 35 percent of the total. The soot generated by the fire can act as an absorber of the radiant energy. Thus, if the fire generates large amounts of soot, the transport of radiant energy through the gas must be calculated in detail [6]. Even in the absence of significant absorption of radiant energy by the products of combustion, the radiant heat transfer to boundaries is an important component of the total heat transfer to any solid surface.

Figure 2 shows a snapshot of the elements used to simulate an isolated fire plume in the absence of any boundaries. Time averages of the output of this kind of simulation must be produced in order to make quantitative comparison with most experimental data. Indeed, it is the fact that the *results* of the simulation can be averaged in a routine way while the *equations* of fluid mechanics cannot is the basis of the whole approach presented here.

On the left of Fig. 3 are the instantaneous vertical centerline velocity and temperature profiles. The oscillations are primarily due to the large toroidal eddies generated at regular intervals at the base of the fire, which then rise asymmetrically. Note that the flow is not even remotely axially symmetric, and the centerline is defined only by the geometry of the pool at the base of the plume. The right side of Fig. 3 shows the corresponding time averaged quantities (solid lines) and McCaffrey's centerline correlations. The *time averaged* flow is symmetric and in excellent agreement with the correlations. The only deviations are at the bottom of the plume where the thermal elements are turned on instantaneously without any preheat as they leave the pool surface, and at the top where the computational "hood" exerts some upstream influence on the plume.

3 Outdoor Fires

Large outdoor fires can be conveniently divided into two categories based on the fuel source. Wildland fires are characterized by a relatively low heat release rate per unit area of ground covered by fuel, but a very large area over which the fire can spread. Indeed, the description of the fire spread process is an essential part of any successful simulation of such an event. Industrial fires, in contrast, are usually much more highly localized but intense emitters of heat, smoke, and other combustion products. This is particularly true if the fuel is a petroleum based substance, with a high energy density and sooting potential. This latter type of fire is the object of study here.

The hazards associated with such fires occur on two widely separated length scales. Near the fire, over distances comparable to the flame length, the radiant energy flux can be sufficiently high to threaten both the structural integrity of neighboring buildings, and the physical safety of firefighters and plant personnel. At much greater distances, typically several times the plume stabilization height in the atmosphere, the smoke and gaseous products generated by the fire can reach the ground in concentrations that may be unacceptable for environmental reasons. The far field hazard has been studied extensively by NIST researchers [7], [8]. This work has led to the development of a computer code ALOFT, which is available from NIST. A comprehensive description of ALOFT and its generalizations to complex terrain can be found in [9].

Consider the near field hazard associated with the flame radiation. The scenario chosen is a fire surrounding an oil storage tank adjacent to several neighboring tanks. This scenario is chosen both for its intrinsic importance and because it illustrates the ingredients needed to generate a realistic simulation of such an event. The heat release generated by a fire on this scale can reach several gigawatts if the entire pool surface is exposed and burning. Such fires interact strongly with the local topography (both natural and man made), and the vertical distribution of wind and temperature in the atmosphere. Moreover, the phenomena are inherently time dependent and involve a wide temperature range. Thus, the simplifications employed in ALOFT and its generalizations can not be used in the present analysis. Indeed, the "low Mach number" combustion equations need to be modified to account for the stratification of the atmosphere.

Figure 4 shows a simulation of a fire resulting from an oil spill trapped in the containment trench surrounding one of the tanks. The diameter of each tank is 84 m, the height 27 m. Each tank is depressed below ground level and surrounded by a containment trench of depth 9 m. The geometry was modeled on the oil storage facility of the Japan National Oil Corporation at Tomokomai, Japan. No attempt was made to represent the entire facility, which contains over 80 tanks. The volume of space represented is a cube

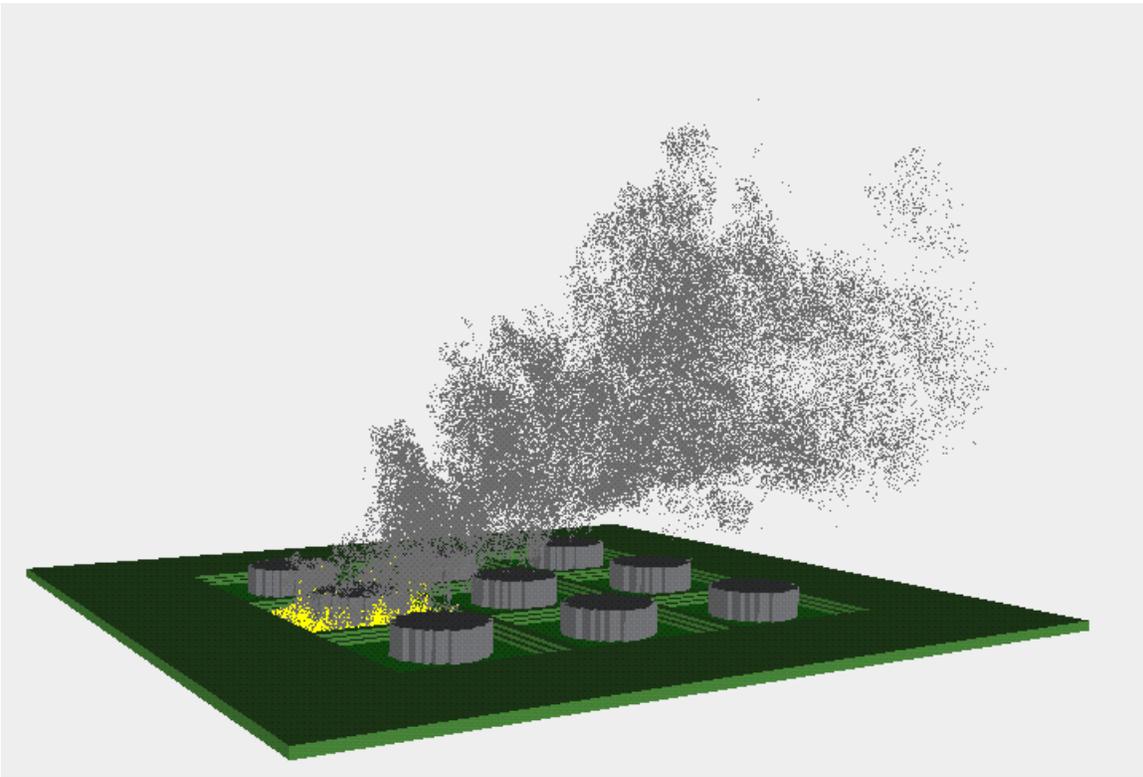


FIGURE 4: Snapshot of oil tank fire simulation with wind speed 6 m/s at the tops of the tanks and the fire in the trench.

768 m on a side. This was filled with a $128 \times 128 \times 128$ array of cells 6 m on a side in the horizontal and ranging from 3 m near the ground to 12 m at the top in the vertical direction. A wind profile that increased from 6 m/s near the tank top to 12 m/s at 768 m that is representative of the atmospheric mean wind profile near the ground was chosen. The ambient temperature was taken to be constant. This is a very stable atmosphere, typical of winter conditions in northern climates. The spilled oil in the trench was assumed to burn with a heat release rate of $1,000 \text{ kW/m}^2$, for a total heat release rate of 12.1 GW. Each element was assumed to emit 35% of its energy as thermal radiation, and 12% of the fuel was converted to soot.

The bright colored elements in fig. 4 are burning, releasing energy into the gas and the radiation field. Thus, the composite burning elements represent the instantaneous flame structure at the resolution limit of the simulation. The dark colored elements are burnt out. They represent the smoke and gaseous combustion products that absorb the radiant energy from the flames. It is important to understand how much of the emitted radiant energy is re-absorbed by the surrounding smoke. The magnitude of this smoke shielding can be realized by computing the radiative flux to the surrounding tanks. A test calculation was performed in which no thermal radiation was absorbed by the smoke. Comparison of the two results showed that the effective radiative fraction reaching the surface is about 6%. Thus, 29% of the original 35% was reabsorbed by the soot. This is consistent with measurements made by Koseki [10]. To explore this further, a separate simulation of a vertical plume in the absence of any wind was performed. The convective energy flux at several heights above the fire bed was calculated. The energy flux was consistently approximately 94% of the total heat release rate in the fire. This means that of the original 35% released as thermal radiation, 29% was reabsorbed, confirming the earlier result. Further details about the model and computations can be found in [11].

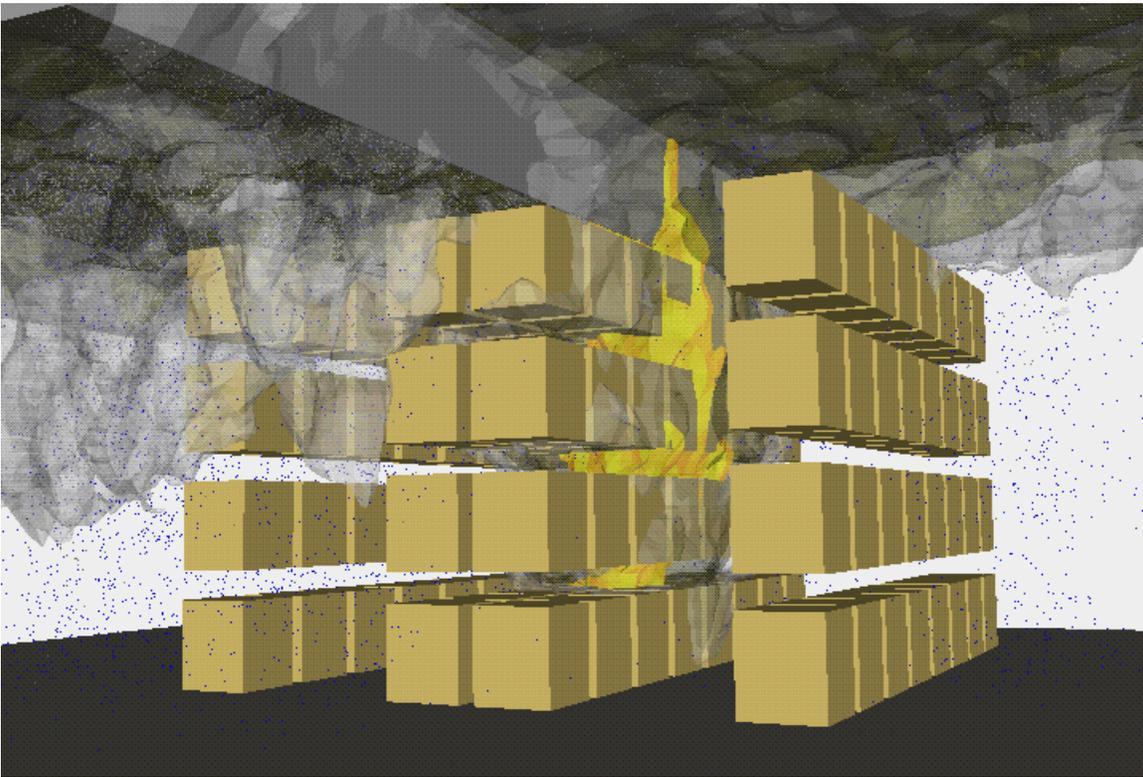


FIGURE 5: Snapshot of large scale fire test simulation showing interaction of sprinkler, draft curtain, and vent in rack storage fire.

4 Industrial Fire Control

Up to this point the emphasis has been on studying fires as natural phenomena. Recently, the LES techniques have begun to be used to study the effects of human intervention to control the damage caused by fires. The International Fire Sprinkler, Smoke and Heat Vent, Draft Curtain Fire Test Project organized by the National Fire Protection Research Foundation brought together a group of industrial sponsors to support and plan a series of large scale tests to study the interaction of sprinklers, roof vents and draft curtains of the type found in large warehouses, manufacturing facilities, and warehouse-like retail stores. The tests were designed to address relatively large, open-area buildings with flat ceilings, sprinkler systems, and roof venting, with and without draft curtains. The most elaborate tests involved a series of five high rack storage commodity burns.

In parallel with the large scale tests, a program was conducted at NIST to develop a computer model based on the LES methodology, the Industrial Fire Simulator (IFS) that incorporated the physical phenomena needed to describe the experiments. A series of bench scale experiments was conducted at NIST to develop necessary input data for the model. These experiments generated data describing the burning rate and flame spread behavior of the cartoned plastic commodity, thermal response parameters and spray pattern of the sprinkler, and the effect of the water spray on the commodity selected for the tests.

Simulations were first compared with heptane spray burner tests, where they were shown to be in good *quantitative* agreement with measured sprinkler activation times and near-ceiling gas temperature rise. The sprinkler activation times were predicted to within 15% of the experimental values for the first ring of sprinklers surrounding the fire, and 25% for the second. The gas temperatures near the ceiling were predicted to within 15%. Next, simulations were performed and compared with the unsprinklered

calorimetry burns of the cartoned plastic commodity. The heat release rates were predicted to within about 20%. Simulations of the 5 cartoned plastic commodity fire tests were then performed. A snapshot from one of the simulations is shown in fig. 5. The goal of these simulations was to be able to differentiate between those experiments that activated a large number of sprinklers and those that did not. This goal has been met. The model was also used to provide valuable insight into what occurred in the experiments, and what would have occurred for various changes of test parameters. Further information about this work can be found in [12], [13].

There are plans to continue the development of the IFS model in the future. Much more work is needed to verify the additional models used to account for the flame spread, the interaction of the spray with fuel surfaces, and the various heat transfer mechanisms. However, the results obtained to date are certainly encouraging. The simulations yield information that is difficult if not impossible to obtain any other way. Moreover, it is possible to test the various assumptions and models individually against experiments designed to yield much more precise information than can be obtained from large scale tests. Thus, the knowledge gained from a limited number of large scale tests could be systematically extended by coupling this information to the results of computer simulations. While this goal has yet to be realized, I do not think it lies all that many years in the future.

Acknowledgments

The work described here is the contribution of many people at NIST. I have been fortunate to have Dr. Ronald Rehm as a collaborator since the beginning of our efforts to develop the capability described above. More recently, Dr. Kevin McGrattan has been the architect and creator of the computer programs that convert the simplified physical and mathematical models into practically useful predictive tools. Dr. William Mell and Mr. William Walton have contributed their expertise as well. Finally, I have been guided and encouraged over the years by my mentor, the Late Prof. Howard W. Emmons, who is certainly the father of modern fire science.

References

- [1] Rehm, R.G. and Baum, H.R., "The Equations of Motion for Thermally Driven, Buoyant Flows", *J. Research of Nat. Bur. Standards*, Vol. 83, pp. 297-308, (1978).
- [2] Baum, H.R., McGrattan, K.B., and Rehm, R.G., "Three Dimensional Simulation of Fire Plume Dynamics", *Fire Safety Science - Proceedings of the Fifth International Symposium*, Y. Hasemi, Ed., International Association for Fire Safety Science, pp. 511-522, (1997).
- [3] McGrattan, K.B., Baum, H.R., and Rehm, R.G., "Large Eddy Simulations of Smoke Movement", *Fire Safety Journal*, Vol. 30, pp. 161-178, (1998).
- [4] Baum, H.R., Ezekoye, O.A., McGrattan, K.B., and Rehm, K.B., "Mathematical Modeling and Computer Simulation of Fire Phenomena", *Theoretical and Computational Fluid Dynamics*, Vol. 6, pp. 125-139, (1994).
- [5] Baum, H.R. and McCaffrey, B.J., "Fire Induced Flow Field - Theory and Experiment", *Fire Safety Science, Proceedings of the Second International Symposium*, Hemisphere, New York, pp. 129-148, (1989).

- [6] Baum, H.R. and Mell, “A radiative transport model for large-eddy fire simulations”, *Combust. Theory Modeling*, Vol. 2, pp. 405-422, (1998).
- [7] Baum, H.R., McGrattan, K.B., and Rehm, R.G., “Simulation of Smoke Plumes from Large Pool Fires”, *Twenty Fifth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, pp. 1463-1469, (1994).
- [8] McGrattan, K.B., Baum, H.R., and Rehm, R.G., “Numerical Simulation of Smoke Plumes from Large Oil Fires”, *Atmospheric Environment*, Vol. 30, pp. 4125-4136, (1996).
- [9] McGrattan, K.B., Baum, H.R., Walton, W.D., and Trelles, J., “Smoke Plume Trajectory from In Situ Burning of Crude Oil in Alaska — Field Experiments and Modeling of Complex Terrain”, NISTIR 5958, National Institute of Standards and Technology, Gaithersburg, (1997).
- [10] Koseki, H. and Mulholland, G.W., “The effect of diameter on the burning of crude oil pool fires,” *Fire Technology*, Vol. 54 (1991).
- [11] Baum, H.R. and McGrattan, K.B., “Simulation of Large Industrial Outdoor Fires”, *Fire Safety Science - Proceedings of the Sixth International Symposium*, to appear.
- [12] McGrattan, K.B., Hamins, A., and Stroup, D., “Sprinkler, Smoke and Heat Vent, Draft Curtain Interaction—Large Scale Experiments and Model Development”, *National Insitute of Standards and Technology NISTIR 6196-1*, (1998).
- [13] McGrattan, K.B., Hamins, A., and Forney, G.P., “Modeling of Sprinkler, Vent and Draft Curtain Interaction”, *Fire Safety Science - Proceedings of the Sixth International Symposium*, to appear.